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Citation for published version:

Oswald, IDH, Motherwell, WDS & Parsons, S 2005, 'Isonicotinamide-formamide (1/1)', *Acta Crystallographica Section E: Structure Reports Online*, vol. 61, pp. O3161-O3163.
<https://doi.org/10.1107/S1600536805026632>

Digital Object Identifier (DOI):

[10.1107/S1600536805026632](https://doi.org/10.1107/S1600536805026632)

Link:

[Link to publication record in Edinburgh Research Explorer](#)

Document Version:

Publisher's PDF, also known as Version of record

Published In:

Acta Crystallographica Section E: Structure Reports Online

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Isonicotinamide–formamide (1/1)

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Key indicators

Single-crystal X-ray study

T = 150 K

Mean $\sigma(\text{C}—\text{C}) = 0.002 \text{ \AA}$

R factor = 0.044

wR factor = 0.122

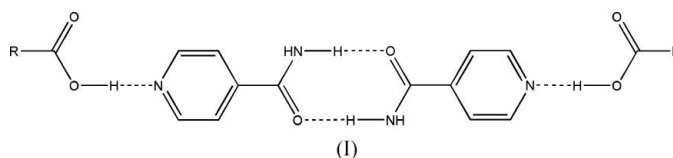
Data-to-parameter ratio = 14.9

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

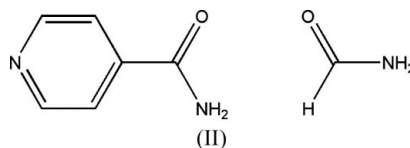
The 1:1 co-crystal of isonicotinamide and formamide, $\text{C}_6\text{H}_6\text{N}_2\text{O} \cdot \text{CH}_3\text{NO}$, consists of hydrogen-bonded dimers, each comprising two isonicotinamide or two formamide molecules. These dimers are connected further by hydrogen bonds into sheets, which are parallel to the $(\bar{2}11)$ plane.

Comment

Isonicotinamide has been shown to crystallize with carboxylic acids in a 1:1 stoichiometry to form a robust building block or 'supermolecule', (I), consisting of two amide and two acid molecules (Aakeröy *et al.*, 2002; Oswald *et al.*, 2004). Amides contain $\text{C}=\text{O}$ and $\text{C}—\text{NH}_2$ groups that could act in an analogous way to the $\text{C}=\text{O}$ and $\text{C}—\text{OH}$ groups of carboxylic acids. The aim of the present investigation was to assess the validity of this analogy in the case of the simplest amide, formamide.



The title co-crystal, (II), crystallizes in the monoclinic space group $P2_1/c$ with one molecule of each component in the asymmetric unit (Fig. 1). The bond distances and angles are unremarkable.



Amides characteristically form $R_2^2(8)$ (Bernstein *et al.* 1995) centrosymmetric dimers through hydrogen bonding between the NH_2 and $\text{C}=\text{O}$ groups. This behaviour is observed in (II), where homomeric dimers are formed (i.e. formamide forms a dimer with another formamide *etc.*), the two components in each case being related by crystallographic inversion centres. The $\text{N} \cdots \text{O}$ distances in the $R_2^2(8)$ dimers are 2.9239 (16) \AA in the case of isonicotinamide and 2.9696 (16) \AA for formamide.

In co-crystals of carboxylic acids with isonicotinamide, homomeric $R_2^2(8)$ dimers are often formed between the amide groups of the isonicotinamide molecules (Aakeröy *et al.*, 2002). The two pyridyl functions at either end of the nicotinamide dimer so formed hydrogen bond to two carboxylic acid

Received 11 July 2005

Accepted 19 August 2005

Online 7 September 2005

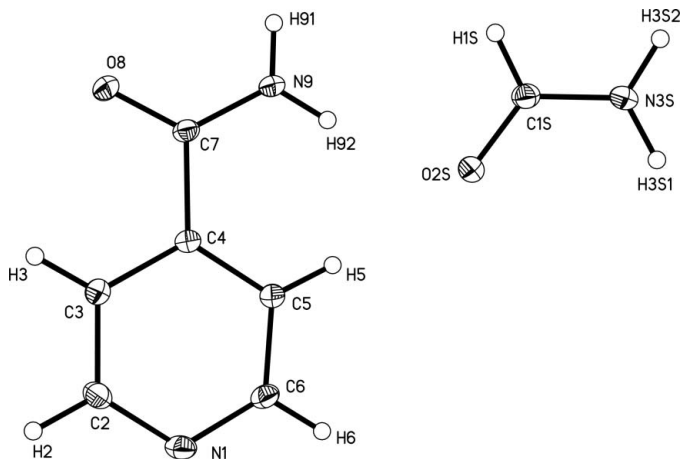


Figure 1
The asymmetric unit of (II). Displacement ellipsoids are shown as 30% probability surfaces and H atoms are drawn as circles of arbitrary radii.

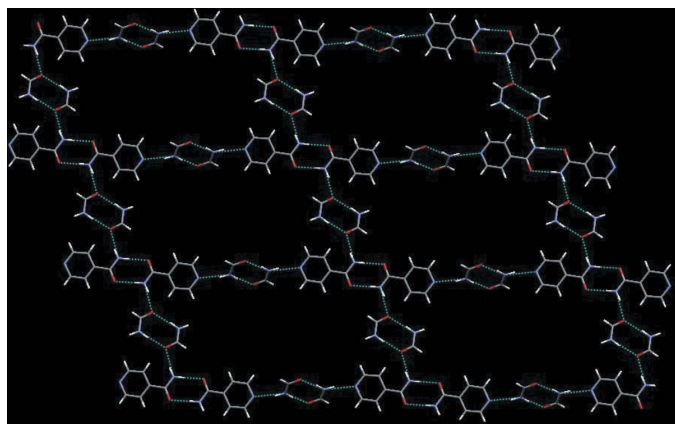


Figure 2
Formation of hydrogen-bonded layers in (II); hydrogen bonds are shown as broken lines. This view is approximately along the $(\bar{2}11)$ reciprocal lattice direction.

molecules in $R_2^2(7)$ motifs comprising C—OH \cdots N and C—H \cdots O hydrogen bonds. Of these interactions, only the $R_2^2(8)$ dimer formation is observed in (II).

The second donor function of the isonicotinamide forms a hydrogen bond to the carbonyl O atom of the formamide; these interactions build up chains. The chains are linked together through a hydrogen bond between a symmetry-equivalent formamide dimer and the pyridine N atom of the isonicotinamide forming an open grid-like layer parallel to the $(\bar{2}11)$ plane (Fig. 2). The second donor function of the formamide molecules serves to link this layer with a symmetry equivalent parallel to $(\bar{2}11)$ filling in the structure.

Experimental

Isonicotinamide (0.49 g, 4.02 mmol) was dissolved in an excess of formamide (1.48 g, 32.10 mmol) and warmed until all the solid dissolved. On cooling, long colourless needles were produced, which fractured into thinner shards, degrading the crystal quality, when attempts were made to cut them to a more suitable length.

Crystal data

$C_6H_6N_2O \cdot CH_3NO$
 $M_r = 167.17$
Monoclinic, $P2_1/c$
 $a = 10.5785$ (18) Å
 $b = 3.7461$ (6) Å
 $c = 20.002$ (3) Å
 $\beta = 94.587$ (3)°
 $V = 790.1$ (2) Å³
 $Z = 4$

$D_x = 1.405$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 1965 reflections
 $\theta = 2.7\text{--}28^\circ$
 $\mu = 0.11$ mm⁻¹
 $T = 150$ (2) K
Needle, colourless
 $1.5 \times 0.14 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)
 $T_{\min} = 0.663$, $T_{\max} = 1.000$
4454 measured reflections

1860 independent reflections
1554 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$
 $\theta_{\max} = 28.7^\circ$
 $h = -13 \rightarrow 10$
 $k = -4 \rightarrow 4$
 $l = -23 \rightarrow 25$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.122$
 $S = 1.06$
1860 reflections
125 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.1905P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.31$ e Å⁻³
 $\Delta\rho_{\min} = -0.20$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N3S-H3S2\cdots N1^i$	0.92 (2)	2.09 (2)	2.9937 (17)	167 (2)
$N3S-H3S1\cdots O2S^{ii}$	0.95 (2)	2.03 (2)	2.9696 (16)	172 (2)
$N9-H91\cdots O8^{iii}$	0.90 (2)	2.03 (2)	2.9239 (16)	172 (2)
$N9-H92\cdots O2S$	0.89 (2)	2.08 (2)	2.9544 (17)	167 (2)
$C5-H5\cdots O2S$	0.95	2.35	3.2384 (17)	156

Symmetry codes: (i) $x, -y + \frac{5}{2}, +z - \frac{1}{2}$; (ii) $-x + 2, -y + 3, -z$; (iii) $-x + 1, -y + 1, -z$.

H atoms attached to C atoms were placed in idealized positions (C—H = 0.95 Å) and allowed to ride on their parent atoms with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$. H atoms attached to N atoms were located in a difference map and refined freely.

Data collection: SMART (Bruker–Nonius, 2001); temperature control: Oxford Cryosystems low-temperature device (Cosier & Glazer, 1986); cell refinement: SAINT (Bruker–Nonius, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 2001) and MERCURY (Taylor & Macrae, 2001; Bruno *et al.*, 2002); software used to prepare material for publication: PLATON (Spek, 2003) and WinGX (Farrugia, 1999).

We thank the CCDC, the EPSRC and The University of Edinburgh for funding.

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